THEORETICAL STUDY OF GROUP 14 $M^+(^2P_J)$-RG COMPLEXES ($M^+ = C^+$, Si^+; RG = He - Ar)

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The light group 14 cations are found in a wide variety of environments, with, for example, C^+ ions thought to play a key role in the chemistry of the interstellar medium,[a] while Si^+ ions are an important component of the upper atmosphere of the Earth due to their presence in meteoroids.[b]

We calculate accurate interatomic potentials for a singly charged carbon cation[c,d] and a singly charged silicon cation[e] interacting with the rare gas atoms helium, neon and argon. The RCCSD(T) method is employed, with basis sets of quadruple-ζ and quintuple-ζ quality, and the energies counterpoise corrected and extrapolated to the basis set limit at each point. In all cases, we consider the lowest electronic states of the M^+ atom, (^2P_J), interacting with the ground electronic state of the RG atom, ($^1S_0$), and compute potentials corresponding to the molecular terms, $^2\Pi$ and $^2\Sigma^+$, as well as the spin-orbit levels which arise: $^2\Pi_{3/2}$, $^2\Pi_{1/2}$ and $^2\Sigma_{1/2}{}^+$. The potentials are employed to calculated spectroscopic constants and ion transport properties.

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[a] S. Petrie and D. K. Bohme, *Mass Spec. Rev.*, **26**, 258 (2007).

[b] J. M. C. Plane, J. C. Gómez-Martin, W. Feng, and D. Janches, *J. Geophys. Res. Atmos.* **121**, 3718 (2016).

[c] W. D. Tuttle, R. L. Thorington, L. A. Viehland and T. G. Wright, *Mol. Phys.* **113**, 3767 (2015).

[d] W. D. Tuttle, R. L. Thorington, L. A. Viehland and T. G. Wright (in preparation).

[e] W. D. Tuttle, R. L. Thorington, L. A. Viehland and T. G. Wright, *Mol. Phys.* **115**, 437 (2017).